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Structural features and the microscopic dynamics of the three-component Zr47Cu46Al7 system: Equilibrium melt, supercooled melt, and amorphous alloy

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Abstract

© 2016, Pleiades Publishing, Inc.The structural and dynamic properties of the three-component Zr47Cu46Al7 system are subjected to a molecular dynamics simulation in the temperature range T = 250–3000 K at a pressure p = 1.0 bar. The temperature dependences of the Wendt–Abraham parameter and the translation order parameter are used to determine the glass transition temperature in the Zr47Cu46Al7 system, which is found to be Tc ≈ 750 K. It is found that the bulk amorphous Zr47Cu46Al7 alloy contains localized regions with an ordered atomic structures. Cluster analysis of configuration simulation data reveals the existence of quasi-icosahedral clusters in amorphous metallic Zr–Cu–Al alloys. The spectral densities of time radial distribution functions of the longitudinal (C̈L(k, ω)) and transverse (C̈T(k, ω)) fluxes are calculated in a wide wavenumber range in order to study the mechanisms of formation of atomic collective excitations in the Zr47Cu46Al7 system. It was found that a linear combination of three Gaussian functions is sufficient to reproduce the (C̈L(k, ω)) spectra, whereas at least four Gaussian contributions are necessary to exactly describe the (C̈T(k, ω)) spectra of the supercooled melt and the amorphous metallic alloy. It is shown that the collective atomic excitations in the equilibrium melt at T = 3000 K and in the amorphous metallic alloy at T = 250 K are characterized by two dispersion acoustic-like branches related with longitudinal and transverse polarizations.

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